

Electronic supplementary information (ESI)

Synthesis and characterization of metal complexes constructed from mixed 4-imidazole-containing ligand and varied multi-carboxylate†

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Table S1 Hydrogen bonding data for complexes **1 - 6**

D-H...A	d(D...A) (Å)	∠D-H...A (°)
Compound 1		
O1W-H1W...O2#1	2.836(2)	172(3)
N2-H2A...O4#2	2.847(2)	169
O1W-H2W...O4	2.662(2)	160(3)
N4-H4A...O3#3	2.821(2)	148
C4-H4...O4#2	3.322(3)	152
C8-H8...O2#2	3.053(2)	130
C12-H12...O1W#4	2.966(3)	111
Compound 2		
N1-H1...O1#5	2.848(3)	162

N3-H3...O4#6	2.676(3)	169
C2-H2...O5#7	3.02(2)	115
C12-H12...O5#8	3.35(3)	171

Compound 3

N2-H2A...O3#9	2.757(4)	147
N3-H3A...O1#10	2.738(4)	150
C8-H8...O2#11	3.324(4)	174
C11-H11...O4#12	3.298(4)	167

Compound 4

N2-H2...O1#13	2.818(4)	164
N4-H4...O4#14	2.799(5)	132
C5-H5...O5#15	3.347(5)	144

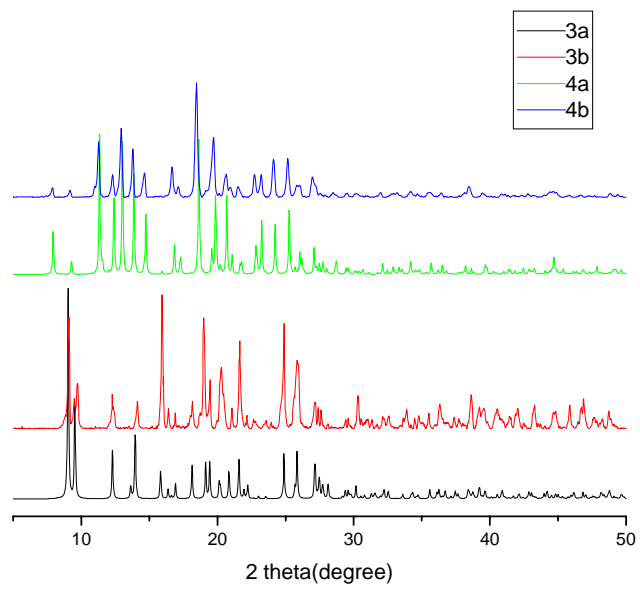
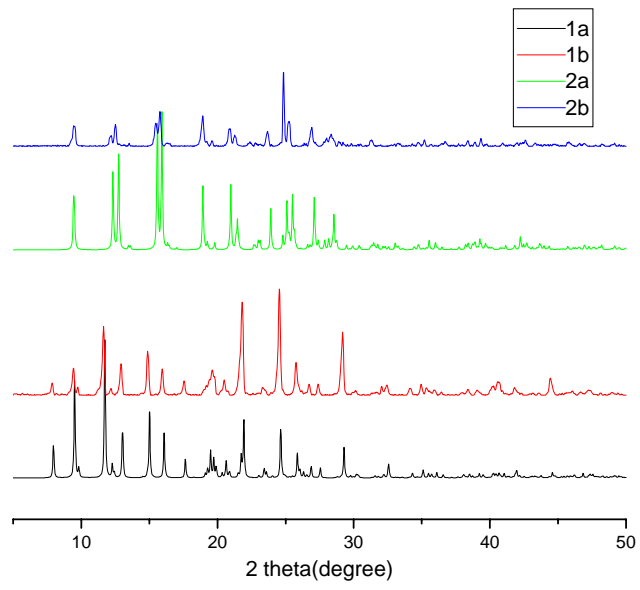
Compound 5

N1-H1A...O1W#16	2.931(4)	173
O1W-H1W...O2#17	2.921(4)	174(4)
O1W-H2W...O3#18	3.120(4)	144(4)
N3-H3A...O2#19	2.751(3)	170
C9-H9...O4#16	3.365(4)	156
C11-H11...O4#16	3.481(4)	164
C12-H12...O2#20	3.158(4)	140

Compound 6

O1W-H1WA...O6#21	2.758(4)	178(2)
O1W-H1WB...O6#22	2.989(4)	154(5)
N2-H2B...O4#23	2.811(3)	151
N4-H4A...O1W#24	2.842(4)	168
C21-H21A...O1#25	3.221(4)	142

Symmetry transformations used to generate equivalent atoms: #1 -x, 1-y, 1-z; #2 -x,1-y,1-z; #3 1-x,1-y,1-z; #4 x,y,-1+z; #5 -x,2-y,-z; #6 x,3/2-y,-1/2+z; #7 1-x,2-y,1-z; #8 1-x,1/2+y,1/2-z; #9 1+x,y,1+z; #10 x,-1+y,z; #11 1-x,-y,1-z; #12 2-x,-y,1-z; #13 1/2+x,1/2-y,-1/2+z; #14 1-x,-y,1-z; #15 1-x,-y,-z; #16 1-x,-y,1-z; #17 -1+x,y,-1+z; #18 1-x,1-y,1-z; #19 -1+x,y,z; #20 2-x,1-y,2-z; #21 x,y,1+z; #22 1-x,-y,1-z; #23 -x,1-y,1-z; #24 1-x,1-y,2-z; #25 1-x,1-y,1-z.



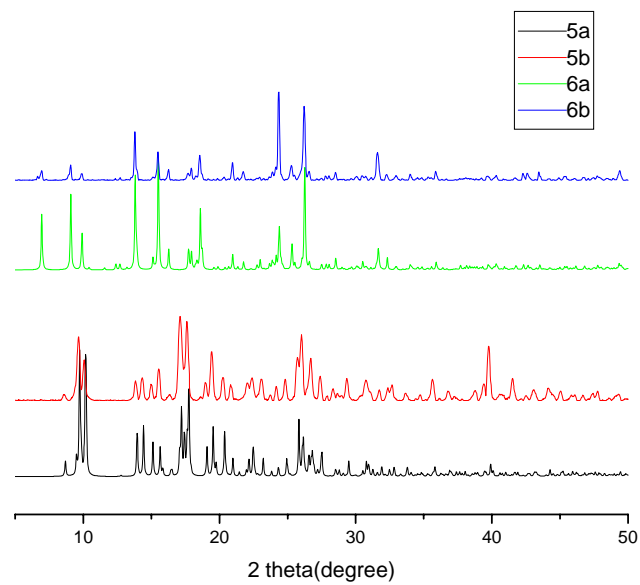


Figure S1. The X-ray powder diffraction patterns of **1 - 6**: a – simulated; b – as-synthesized.

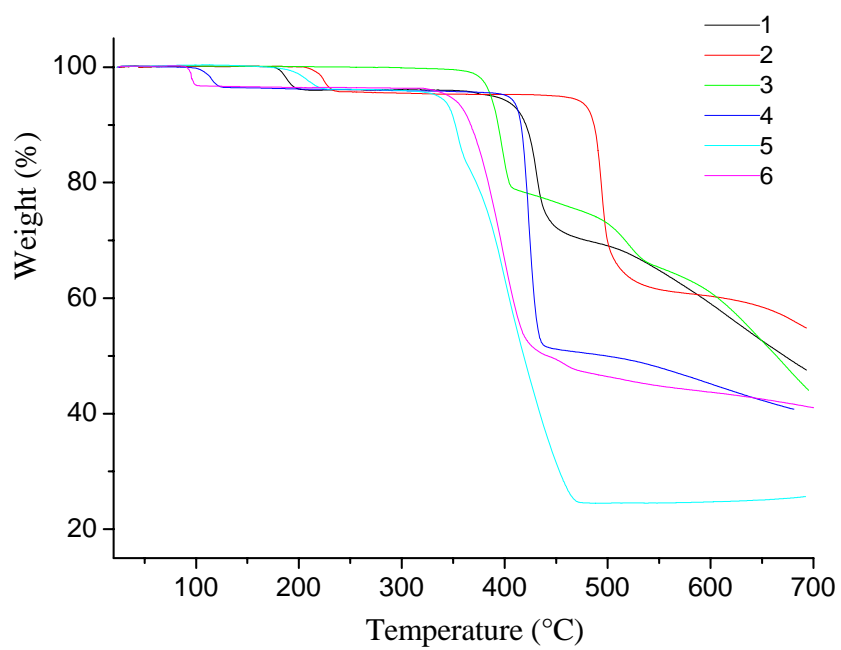


Figure S2. The TG curves of **1 - 6**.

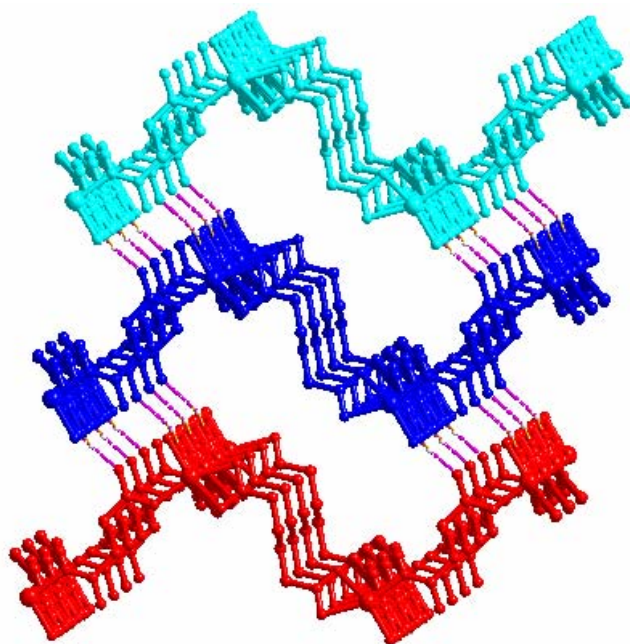


Figure S3. 3D framework of **1** linked by hydrogen bonds indicated by dashed line.

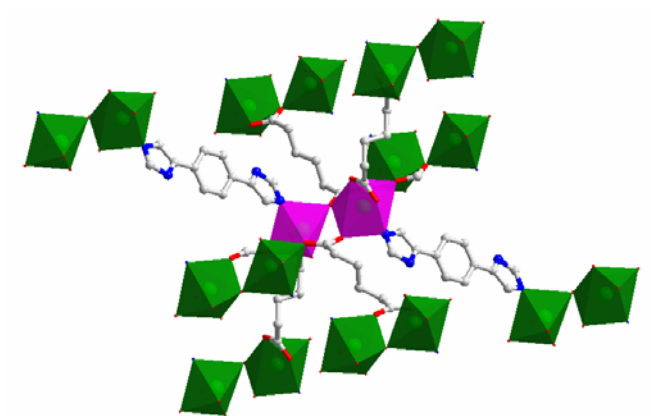


Figure S4. View of the linkages of a binuclear Cd(II) nodes (purple) with eight adjacent cores (green) of **3**.

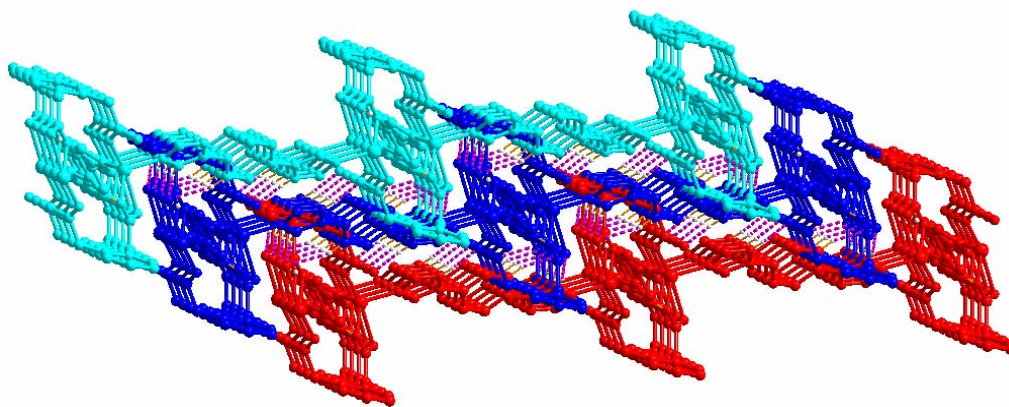


Figure S5. 3D framework of **5** linked by hydrogen bonds indicated by dashed line.

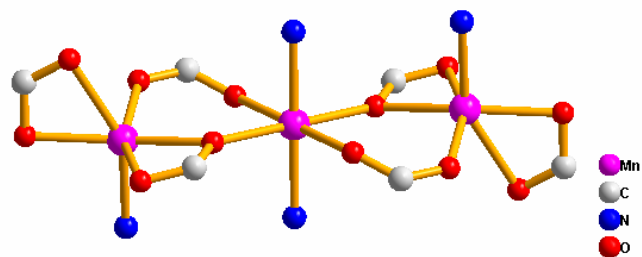


Figure S6. The Mn₃-based SBUs [Mn₃(CO₂)₆N₄] of **6**.

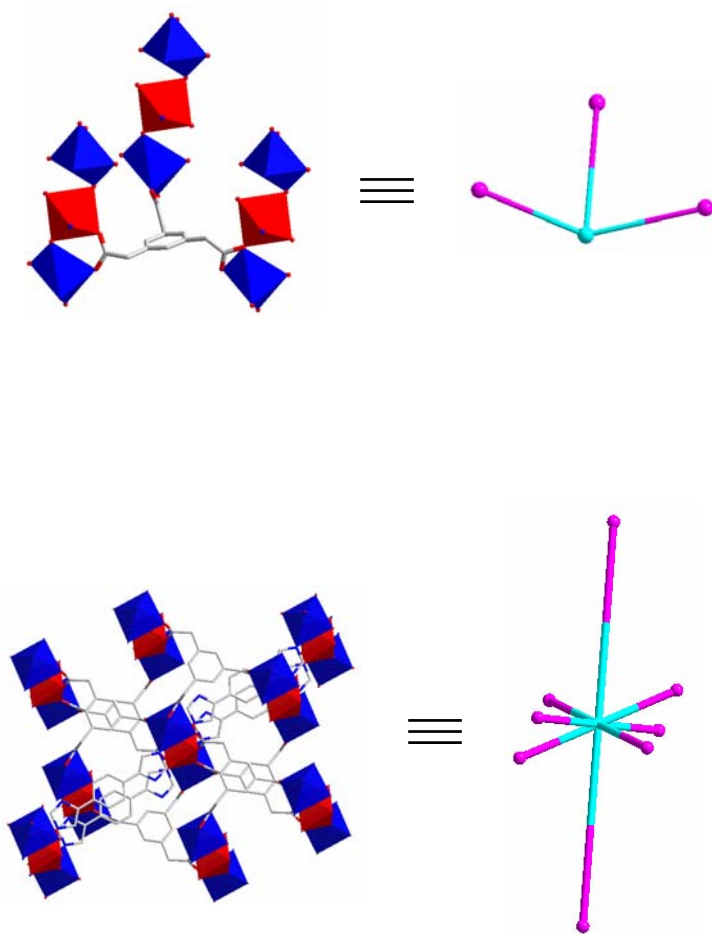


Figure S7. Ball-and-stick and polyhedral representations of the 3-connected bta³⁻ ligand and 8-connected trinuclear Mn(II) cluster of **6**.